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Dr. Judah Goldwasser

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## COMPUTED HEATS OF FORMATION

by

Peter Politzer, M. Edward Grice, Monica C. Concha and Pat Lane

Department of Chemistry University of New Orleans New Orleans, LA 70148

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Unlimited distribution  13. ABSTRACT (Maximum 200 words)  NO2  NO2  NO2  NO2  NO4  NO2  NO5  NO5  NO6  NO6  NO6  NO7  NO7  NO7  NO7  NO7	Computed he $O_2$ $O_2N - N$ $O_$	3: $Z = H$ 4: $Z = N$ NO <sub>2</sub> 5: $Z = N$ (solid) = 231 cal/g (solid) = 491 cal/g (solid) = 150 cal/g	O <sub>2</sub> $O_2N$ $O_$
Unlimited distribution  13. ABSTRACT (Maximum 200 words)  NO2  NO2  NO2  NO2  NO2  NO2  NO2	Computed he compu	3: $Z = H$ 4: $Z = N$ NO <sub>2</sub> 5: $Z = N$ (solid) = 231 cal/g (solid) = 491 cal/g (solid) = 150 cal/g	O <sub>2</sub> $O_2N \longrightarrow N-N \longrightarrow NO_2$ 6  5: $\Delta H_f^{298K}$ (solid) = 132 cal/8  6: $\Delta H_f^{298K}$ (solid) = 235 cal/8  7: $\Delta H_f^{298K}$ (solid) = 1.5 cal/8  8: $\Delta H_f^{298K}$ (solid) = -584 cal/
Unlimited distribution  13. ABSTRACT (Maximum 200 words)  NO2  NO2  NO2  NO2  NO4  NO5  NO5  NO5  NO5  NO5  NO5  NO5	Computed he compu	3: $Z = H$ 4: $Z = N$ NO <sub>2</sub> 5: $Z = N$ (solid) = 231 cal/g (solid) = 491 cal/g (solid) = 150 cal/g	O <sub>2</sub> $O_2N$ $N-N$ $O_2$ $O_2N$ $N-N$ $O_2$ $O_2N$

We have computed heats of formation for compounds 1 - 8 (Table 1). The first five are target compounds proposed by M. Trudell (University of New Orleans); 6 - 8 have recently been prepared by R. Schmitt and J. Bottaro (SRI). For the molecular systems 1 - 7, we used our density functional procedure to obtain gas phase heats of formation, which were converted to liquid and solid state values by subtracting, respectively, the heats of vaporization and sublimation. The latter are determined by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [2,3]. (Vibrational energies were obtained from the molecular stoichiometries [4].) For the ionic solid 8, the heat of formation was calculated using the lattice enthalpy and the gas phase heats of formation of the positive and negative ions; the lattice enthalpy was computed from our recently-developed relationship involving anionic surface electrostatic potentials [5]. For comparison, the experimental solid phase heats of formation of HMX and RDX are, respectively, 60.4 cal/g and 76.1 cal/g [6].

## References:

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 $\begin{array}{c}
1 \\
0 \\
N
\end{array}$   $\begin{array}{c}
NO_2 \\
N\\
NO_2
\end{array}$   $\begin{array}{c}
NO_2 \\
NO_2
\end{array}$ 

 $\Delta H_f^{298K} (gas) = 73.6 \text{ kcal/mole} = 341 \text{ cal/g}$   $\Delta H_f^{298K} (\text{liquid}) = 60.0 \text{ kcal/mole} = 278 \text{ cal/g}$   $\Delta H_f^{298K} (\text{solid}) = 49.8 \text{ kcal/mole} = 231 \text{ cal/g}$ 

$$\begin{split} \Delta H_f^{298K} \left( gas \right) &= 155 \text{ kcal/mole} = 604 \text{ cal/g} \\ \Delta H_f^{298K} \left( \text{liquid} \right) &= 139 \text{ kcal/mole} = 544 \text{ cal/g} \\ \Delta H_f^{298K} \left( \text{solid} \right) &= 126 \text{ kcal/mole} = 491 \text{ cal/g} \end{split}$$

 $\Delta H_f^{298K} (gas) = 80.6 \text{ kcal/mole} = 263 \text{ cal/g}$   $\Delta H_f^{298K} (liquid) = 64.3 \text{ kcal/mole} = 210 \text{ cal/g}$   $\Delta H_f^{298K} (solid) = 45.8 \text{ kcal/mole} = 150 \text{ cal/g}$ 

4 
$$O_2N NO_2$$
  $O_2N^{NO_2}$   $O_2N^{NO_2}$   $O_2N^{NO_2}$   $O_2N^{NO_2}$ 

 $\Delta H_f^{298K} (gas) = 104 \text{ kcal/mole} = 264 \text{ cal/g}$   $\Delta H_f^{298K} (liquid) = 87.5 \text{ kcal/mole} = 221 \text{ cal/g}$   $\Delta H_f^{298K} (solid) = 62.2 \text{ kcal/mole} = 157 \text{ cal/g}$ 

 $\Delta H_f^{298K} (gas) = 96.5 \text{ kcal/mole} = 236 \text{ cal/g}$   $\Delta H_f^{298K} (liquid) = 79.1 \text{ kcal/mole} = 194 \text{ cal/g}$   $\Delta H_f^{298K} (solid) = 54.0 \text{ kcal/mole} = 132 \text{ cal/g}$ 

 $\Delta H_f^{298K}$  (gas) = 108 kcal/mole = 370 cal/g  $\Delta H_f^{298K}$  (liquid) = 91.1 kcal/mole = 312 cal/g  $\Delta H_f^{298K}$  (solid) = 68.7 kcal/mole = 235 cal/g

(continued)

Table 1. Computed heats of formation (continued).

7 
$$O_2N$$
  $N-F$ 

$$\begin{split} \Delta H_f^{298K}\left(gas\right) &= 20.5 \text{ kcal/mole} = 124 \text{ cal/g} \\ \Delta H_f^{298K}\left(\text{liquid}\right) &= 8.23 \text{ kcal/mole} = 49.8 \text{ cal/g} \\ \Delta H_f^{298K}\left(\text{solid}\right) &= 0.24 \text{ kcal/mole} = 1.5 \text{ cal/g} \end{split}$$

$$\Delta H_f^{298K}$$
 (solid) = -69.0 kcal/mole = -584 cal/g